Oxazole

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 95.4 °C

Global applicability domain: Inside

Local applicability domain index: 6.26e-01

Confidence level: 7.22e-01

Nearest Neighbors from the Training Set

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Oxazole
Measured: 69.5
Predicted: 95.4

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Isoxazole
Measured: 95.0
Predicted: 86.9

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1-Propene, 3-nitro-
Measured: 128
Predicted: 125

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4-Methyloxazole
Measured: 88.0
Predicted: 100